Structure of R-salbutamol Sulfate

S. Pagola, P. Stephens (Physics & Astronomy, SUNY, Stony Brook,) and S. Cuffini (CEPROCOR, Córdoba, Argentina)

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Beamline(s): **X3B1**

Introduction: Salbutamol is a drug used in asthma therapy. The single enantiomer, R-salbutamol, has desirable bronchodilatator, bronchoprotective and anti-edematous properties. However, racemic salbutamol can intensify allergic bronchospasm and promote eosinophil activation in asthmatic airways [1].

The crystal structure of the racemic mixture has been previously determined [2] by single crystal X-ray diffraction. We have characterized the crystal structure of R-salbutamol sulfate, using high resolution X-ray powder diffraction.

Methods and Materials: The X-ray powder diffraction pattern of a sample of R-salbutamol sulfate was collected at X3B1 beamline in a capillary. The pattern was indexed using the program ITO [3], and a Le Bail fit was done using FULLPROF [4]. A strong candidate structure was found with our program PSSP [5].

Results: The powder pattern was indexed to the monoclinic cell a=28.084(3) Å, b=6.1428(7) Å, c=16.502(2) Å, α=90°, β=95.534(7)°, γ=90°, cell volume=2833.5(5) Å^3. The space group C 2 is consistent with the systematic absences observed. As the racemic mixture, the material has two inequivalent salbutamol molecules in the asymmetric unit and a sulfate ion. Each R-salbutamol molecule has 5 torsions. Thus, 28 structural parameters to locate the molecules and determine the conformations were calculated. This is substantially more complex than other structures solved at present using simulated annealing methods. Since the number of potential false minima increases rapidly with structural complexity, more work is required to verify that this is the correct solution.

After Rietveld refinement of a candidate structure, R_{wp}=15.6% and R_I=6.8%. The structure is shown in **Figure 1**.

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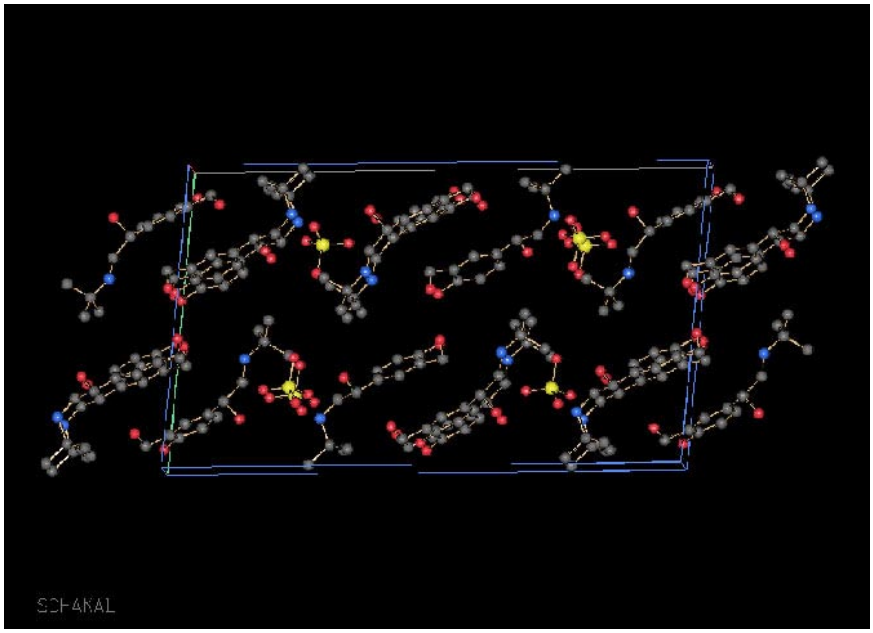

Figure 1. Representation of the structure of R-Salbutamol sulfate along [010].